Spin-Orbit Split Surface States on Li/W(110)

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In a recent study of the surface bands of W(110) in the presence of hydrogen[1], we found a disagreement between the predicted and observed number of surface states on the clean and hydrogen-covered W(110) surfaces. Figure 1 shows bandmapping and fermi contour results from that study, in this case for 1 monolayer of hydrogen on W(110). In fig. 1(a), we see a series of angle-resolved valence band photoemission spectra acquired as a function of polar emission angle θ. By converting θ to k sin θ, we have converted the angle axis directly into electron momentum $k_{\|}$ parallel to the surface. Ignoring the emission near the center of Fig. 1(a) (which is due to unimportant bulk transitions), we see two well-defined, parabolic bands of similar intensity.

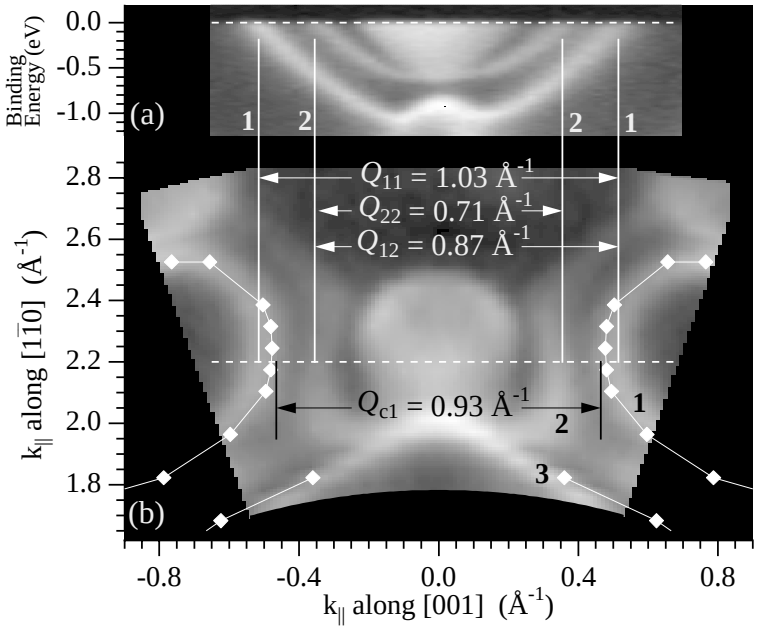

Figure 1. Angle-resolved photoemission results for 1 monolayer of hydrogen on W(110). (a) Valence bandmaps along a line in $k_{\|}$-space. (b) Fermi contours over the $k_{\|}$-plane. The intensity along the dashed lines in (a) and (b) are along the same line in the two -dimensional $k_{\|}$-plane. The vectors Q_{ij} arerelated to electron-phonon coupling, and are discussed in Ref. 1.

To illustrate the momentum-dependence of these states further, consider the photoemission intensity at the Fermi level E_f (zero binding energy). Intensity acquired along the dashed line in Fig. 1(a), which comprises a line in two-dimensional $k_{\|}$-space, may be acquired in other directions in the $k_{\|}$-plane. Such an intensity map, called a Fermi contour map, is shown in fig. 1(b). For comparison, the dashed line in fig. 1(b) corresponds to the same dashed line in fig. 1(a). In the fermi contour map in fig. 1(b), contours labeled 1 and 2 correspond to the two bands seen in fig. 1(a).

Also shown in fig. 1(b) is a recent calculation by Kohler et al.[2] (diamonds), This calculation finds a similar contour to our contour #1, but misses contour #2. The spin-orbit interaction is a relativistic effect expected to be important for W, and is the only relativistic effect not included in the (scalar relativistic) calculation. To test whether the splitting is due to such relativisitic effects, we have performed a comparison study of H on Mo, as well as the similar systems Li on Mo(110) and Li on W(110). Because of the lighter atomic mass of Mo, relativistic effects should be considerably less important on this surface.

Figure 2 shows Fermi contour maps for Li/W compared to Li on Mo. These maps are over a more extensive region of k-space; for comparison the region in fig. 1(b) corresponds to the

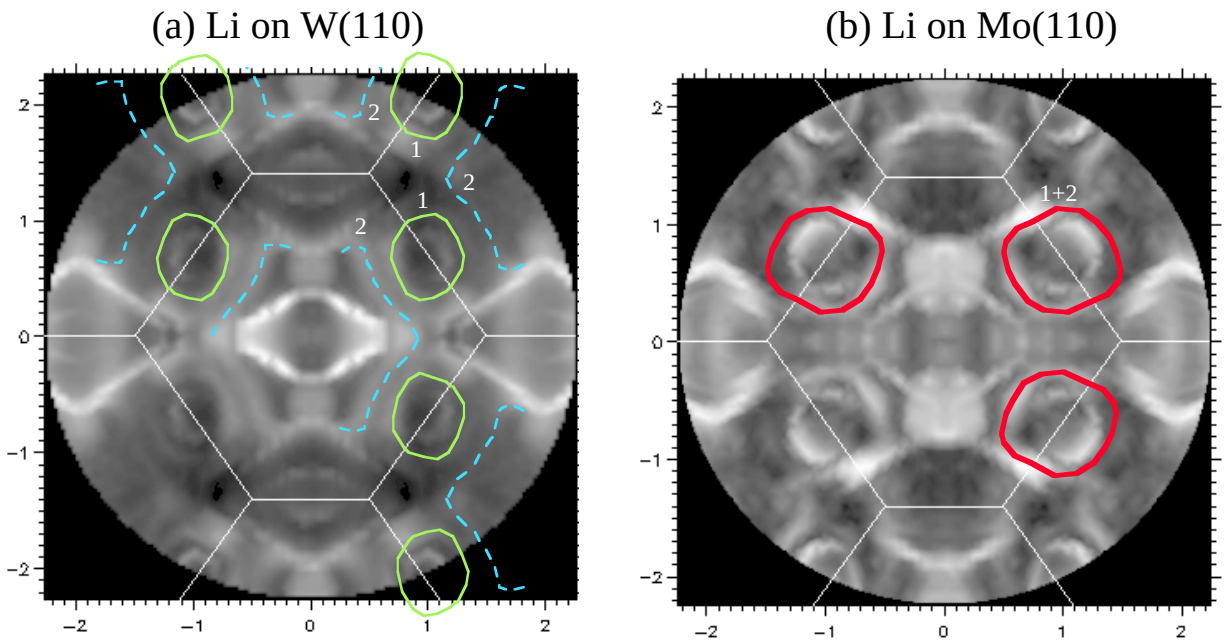

Figure 2. Fermi contour maps for (a) Li on W(110) and (b) Li on Mo(110). The two orbits "1" and "2" in (a) correspond to the single orbit "1+2" in (b),

region at the tops of fig. 2(a-b). Since Li and H have similar outer valence electrons, the results from Li on W are similar to those from H on W: there is a similar pair of Fermi contours, labelled "1" and "2", in fig. 2(a). By changing the substrate from W to Mo, very little should be changed, since W and Mo have the same valence and lattice constants. The most significant difference is the removal of spin-orbit as well as other relativistic interactions. In fig. 2(b), we see the results for Mo. These are very similar to W except that where two orbits "1" and "2" exist for W, we find only a single orbit "1+2" for Mo. Upon more detailed investigation we found that orbit 1+2 for Mo is indeed slightly split at energies below the Fermi level. At the Fermi level, however, the splitting becomes unresolvable.

Recently, a strikingly similar splitting of the surface Fermi contours was observed in the clean Au(111) surface state at zone center,[3] which is not observed either for Ag(111) or Cu(111). In that study, the authors found that a simple model for the spin-orbit interaction could account for the magnitude of the splittings, as well as predict that the spin ordering was in-plane along the tangents of the Fermi contours. In that case, however, the theory was simplified by the near spherical symmetry of the *sp*-derived wavefunctions near zone center. In our case, we have the additional complications that the surface states are far from zone center and are derived from *d* states. Therefore, we cannot apply such a simple theory to determine the spin ordering. The magnitudes of the shifts in energy, however, are consistent with atomic spin-orbit splittings seen in Mo and W in analogy with Ag and Au. It would be interesting to explore this system further theoretically as well as experimentally—perhaps using spin-resolved detection—to more directly confirm that spin-orbit interaction is responsible.

REFERENCES

[1]E. Rotenberg and S. D. Kevan, Phys. Rev. Lett., in press.
[2]B. Kohler, P. Ruggerone, M. Scheffler, Phys. Rev. B. **56**, 13 503 (1997).
[3]S. LaShell, B. A. McDougall, and E. Jensen, Phys. Rev. Lett. **77**, 3419 (1996).

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